

Simulation of Neutron and Gamma Ray Emission from Fission

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1 Data and physics models

This paper describes a general-purpose and extensible software library to accurately simulate neutron and gamma-ray emission from fission reactions (both spontaneous and neutron induced). This was motivated by detailed statistical studies of fission chains in multiplying media. This model is data-driven and incorporates all available multiplicity measurements found in the literature. Empirical models are employed whenever multiplicity data are not available. Essentially no data are available for the correlations between the neutrons and gammas, so this model samples these distributions independently. By default, this model effectively scales the multiplicity data to match the average multiplicity value ($\bar{\nu}$) found in external evaluated data libraries. At present the gammas and neutrons are emitted isotropically. The data and empirical models are described in detail in the following subsections. This model has been incorporated into the latest release of Geant4 and has been submitted for inclusion in future versions of MCNPX and COG. The standalone version of the software library can be downloaded from <http://nuclear.llnl.gov/simulation>.

1.1 Neutron number distribution

Based on reasonable assumptions about the distribution of excitation energy among fission fragments, Terrell [1] showed that the probability P_ν of observing ν neutrons from fission can be approximated by a Gaussian-like distribution

$$\sum_{n=0}^{\nu} P_n = \frac{1}{2\pi} \int_{-\infty}^{\frac{\nu - \bar{\nu} + \frac{1}{2} + b}{\sigma}} e^{-\frac{t^2}{2}} dt \quad (1)$$

where $\bar{\nu}$ is the average number of neutrons, σ (set to 1.079) is the width of the distribution, and b is a small correction factor ($b < 0.01$) that ensures that the discrete probability distribution has the correct average $\bar{\nu}$. This model is used when no explicit multiplicity data are available.

Neutron-induced fission data

Zucker and Holden [3] measured the neutron multiplicity distributions for ^{235}U , ^{238}U , and ^{239}Pu (see Tables 1-3), as a function of the incident neutron energy E_n from zero through ten MeV in increments of one MeV. Fig. 1 shows the neutron number distribution for induced fission of ^{235}U . Gwin, Spencer and Ingle [4] measured the distribution at thermal energies for ^{235}U . In addition, there are many measurements of $\bar{\nu}$, the average number of emitted neutrons, for many isotopes. Since there are multiple methods for parameterizing the multiplicity data and renormalizing the overall distributions to agree with the specific measured values of $\bar{\nu}$, we provide four options for generating neutron multiplicity distributions. These options are selected by the internal variable `nudist`, default=3.

The first option (`nudist=0`) uses a fit to the Zucker and Holden data [3] by Valentine [5] [6]. Valentine expressed the P_ν 's (for $\nu = 0, \dots, 8$) as 5th order polynomials in E_n , the incident neutron energy. These functions $P_\nu(E_n)$ are used to sample the neutron multiplicity for E_n in the range 0 to 10 MeV. When E_n is greater than 10 MeV, $E_n=10$ MeV is used to generate P_ν .

In addition to using the Zucker and Holden data above for incident neutron energies E_n above 1 MeV, the second option (`nudist=1`) also uses the Gwin, Spencer and Ingle data [4] for ^{235}U at thermal energies (0 MeV) to generate $P_\nu(E_n)$ polynomials. As in the first option, when E_n is greater than 10 MeV, $E_n=10$ MeV is used to generate P_ν .

The third option (`nudist=2`) implements an alternative polynomial fit from Valentine [6] of P_ν as a function of $\bar{\nu}$ instead of E_n , following the suggestion of Frehaut [7]. When a neutron induces a fission, the

E_n	$\nu=0$	1	2	3	4	5	6	7	$\bar{\nu}$
0	.0317223	.1717071	.3361991	.3039695	.1269459	.0266793	.0026322	.0001449	2.4140000
1	.0237898	.1555525	.3216515	.3150433	.1444732	.0356013	.0034339	.0004546	2.5236700
2	.0183989	.1384891	.3062123	.3217566	.1628673	.0455972	.0055694	.0011093	2.6368200
3	.0141460	.1194839	.2883075	.3266568	.1836014	.0569113	.0089426	.0019504	2.7623400
4	.0115208	.1032624	.2716849	.3283426	.2021206	.0674456	.0128924	.0027307	2.8738400
5	.0078498	.0802010	.2456595	.3308175	.2291646	.0836912	.0187016	.0039148	3.0386999
6	.0046272	.0563321	.2132296	.3290407	.2599806	.1045974	.0265604	.0056322	3.2316099
7	.0024659	.0360957	.1788634	.3210507	.2892537	.1282576	.0360887	.0079244	3.4272800
8	.0012702	.0216090	.1472227	.3083032	.3123950	.1522540	.0462449	.0107009	3.6041900
9	.0007288	.0134879	.1231200	.2949390	.3258251	.1731879	.0551737	.0135376	3.7395900
10	.0004373	.0080115	.1002329	.2779283	.3342611	.1966100	.0650090	.0175099	3.8749800

Table 1: Neutron number distribution for induced fission in ^{235}U .

E_n	$\nu=0$	1	2	3	4	5	6	7	8	$\bar{\nu}$
0	.0396484	.2529541	.2939544	.2644470	.1111758	.0312261	.0059347	.0005436	.0001158	2.2753781
1	.0299076	.2043215	.2995886	.2914889	.1301480	.0363119	.0073638	.0006947	.0001751	2.4305631
2	.0226651	.1624020	.2957263	.3119098	.1528786	.0434233	.0097473	.0009318	.0003159	2.5857481
3	.0170253	.1272992	.2840540	.3260192	.1779579	.0526575	.0130997	.0013467	.0005405	2.7409331
4	.0124932	.0984797	.2661875	.3344938	.2040116	.0640468	.0173837	.0020308	.0008730	2.8961181
5	.0088167	.0751744	.2436570	.3379711	.2297901	.0775971	.0225619	.0030689	.0013626	3.0513031
6	.0058736	.0565985	.2179252	.3368863	.2541575	.0933127	.0286200	.0045431	.0031316	3.2064881
7	.0035997	.0420460	.1904095	.3314575	.2760413	.1112075	.0355683	.0065387	.0031316	3.3616731
8	.0019495	.0309087	.1625055	.3217392	.2943792	.1313074	.0434347	.0091474	.0046284	3.5168581
9	.0008767	.0226587	.1356058	.3076919	.3080816	.1536446	.0522549	.0124682	.0067176	3.6720432
10	.0003271	.0168184	.1111114	.2892434	.3160166	.1782484	.0620617	.0166066	.0095665	3.8272281

Table 2: Neutron number distribution for induced fission in ^{238}U .

algorithm converts the incident neutron energy E_n into $\bar{\nu}$ using conversion tables (typically ENDF/EDNL), generates the P_ν distributions for that value of $\bar{\nu}$, and then samples the P_ν distributions to determine ν . The least-square fits to the ^{235}U data are used for both ^{235}U and ^{233}U neutron induced fission, the fits to ^{238}U are used for ^{232}U , ^{234}U , ^{236}U and ^{238}U , while the fits to ^{239}Pu are used for ^{239}Pu and ^{241}Pu . Data comes from Zucker and Holden. For ^{235}U , data comes from Zucker and Holden for E_n greater than 1 MeV, and Gwin, Spencer and Ingle for 0 MeV. The fits are only used when $\bar{\nu}$ is in the range of the $\bar{\nu}$'s for the tabulated data. Otherwise, Terrell's approximation is used.

The fourth option, which is the default (nudist=3), is similar to the third option except that the P_ν distributions are not functions of $\bar{\nu}$, but are left intact as multiplicity distributions for the data listed in Gwin, Spencer and Ingle, and for the data listed in Zucker and Holden. The multiplicity distribution P_ν from which the number of neutrons will be sampled is selected based on the value of $\bar{\nu}$ for a given induced fission event. For instance, if $P_\nu(1\text{MeV})$ has $\bar{\nu} = 2.4$, $P_\nu(2\text{MeV})$ has $\bar{\nu} = 2.6$, and $\bar{\nu}$ is 2.45 at the energy of the incident fission-inducing neutron (this value $\bar{\nu}$ comes typically from cross-section data libraries such as ENDF/ENDL), the probability of sampling the number of neutrons ν from $P_\nu(1\text{MeV})$ and $P_\nu(2\text{MeV})$ will be 25% and 75%, respectively. This technique is only used when $\bar{\nu}$ is in the range of the $\bar{\nu}$'s for the tabulated data. Otherwise, Terrell's approximation is used. This last way of computing ν has several advantages: first, the data as listed in the original papers is used exactly, as opposed to approximated by low-ordered polynomials least-square fitting the original data. Second, the data from the Gwin, Spencer and Ingle paper, and the data from the Zucker and Holden paper is entered as-is as a table in the code, and can

E_n	$\nu=0$	1	2	3	4	5	6	7	8	$\bar{\nu}$
0	.0108826	.0994916	.2748898	.3269196	.2046061	.0726834	.0097282	.0006301	.0001685	2.8760000
1	.0084842	.0790030	.2536175	.3289870	.2328111	.0800161	.0155581	.0011760	.0003469	3.0088800
2	.0062555	.0611921	.2265608	.3260637	.2588354	.0956070	.0224705	.0025946	.0005205	3.1628300
3	.0045860	.0477879	.1983002	.3184667	.2792811	.1158950	.0301128	.0048471	.0007233	3.3167800
4	.0032908	.0374390	.1704196	.3071862	.2948565	.1392594	.0386738	.0078701	.0010046	3.4707300
5	.0022750	.0291416	.1437645	.2928006	.3063902	.1641647	.0484343	.0116151	.0014149	3.6246800
6	.0014893	.0222369	.1190439	.2756297	.3144908	.1892897	.0597353	.0160828	.0029917	3.7786300
7	.0009061	.0163528	.0968110	.2558524	.3194566	.2134888	.0729739	.0213339	.0020017	3.9325800
8	.0004647	.0113283	.0775201	.2335926	.3213289	.2356614	.0886183	.0274895	.0039531	4.0865300
9	.0002800	.0071460	.0615577	.2089810	.3200121	.2545846	.1072344	.0347255	.0054786	4.2404900
10	.0002064	.0038856	.0492548	.1822078	.3154159	.2687282	.1295143	.0432654	.0075217	4.3944400

Table 3: Neutron number distribution for induced fission in ^{239}Pu .

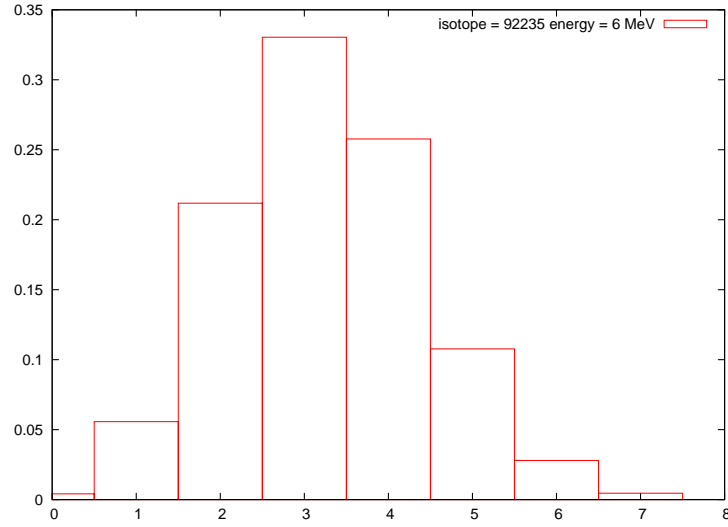


Figure 1: Induced fission in ^{235}U , incident neutron energy = 6MeV

easily be checked and maintained if necessary by the application developer. Third the method provides a simple and statistically correct mechanism of sampling the data tables. The fission module behaves in this manner when the 'nudist' option is set to 3, which is also the default behavior.

Spontaneous fission data

For ^{252}Cf , the fission module can be set to use either the measurements by Spencer [8] ($\text{ndist}=0$), which is the default, or Boldeman [9] ($\text{ndist}=1$).

For ^{238}U , ^{240}Pu , ^{242}Pu , ^{242}Cm , ^{244}Cm , the probability distribution data comes from Holden and Zucker [10], while for ^{236}Pu and ^{238}Pu , it comes from Santi et al. [11] The measured data is summarized in Table 4.

If no full multiplicity distribution data exists, the fission module uses Terrell [1]'s approximation with $\bar{\nu}$ from Ensslin [12]. The measured values from Ensslin are listed in Table 5.

isotope	$\nu=0$	1	2	3	4	5	6	7	8	9
^{238}U	.0481677	.2485215	.4253044	.2284094	.0423438	.0072533	0	0	0	0
^{236}Pu	.0802878	.2126177	.3773740	.2345049	.0750387	.0201770	0	0	0	0
^{238}Pu	.0562929	.2106764	.3797428	.2224395	.1046818	.0261665	0	0	0	0
^{242}Pu	.0679423	.2293159	.3341228	.2475507	.0996922	.0182398	.0031364	0	0	0
^{242}Cm	.0212550	.1467407	.3267531	.3268277	.1375090	.0373815	.0025912	.0007551	.0001867	0
^{244}Cm	.0150050	.1161725	.2998427	.3331614	.1837748	.0429780	.0087914	.0002744	0	0
^{252}Cf [8]	.00211	.02467	.12290	.27144	.30763	.18770	.06770	.01406	.00167	.0001
^{252}Cf [9]	.00209	.02621	.12620	.27520	.30180	.18460	.06680	.01500	.00210	0

Table 4: Neutron number distribution for spontaneous fission.

isotope	$\bar{\nu}$	a	b
^{232}Th	2.14	1.25	4.0
^{232}U	1.71	1.12082	3.72278
^{233}U	1.76	1.16986	4.03210
^{234}U	1.81	1.29661	4.92449
^{235}U	1.86	1.29080	4.85231
^{236}U	1.91	1.36024	5.35746
^{238}U	2.01	1.54245	6.81057
^{237}Np	2.05	1.19985	4.24147
^{238}Pu	2.21	1.17948	4.16933
^{239}Pu	2.16	1.12963	3.80269
^{240}Pu	2.156	1.25797	4.68927
^{241}Pu	2.25	1.18698	4.15150
^{242}Pu	2.145	1.22078	4.36668
^{241}Am	3.22	1.07179	3.46195
^{242}Cm	2.54	1.12695	3.89176
^{244}Cm	2.72	1.10801	3.72033
^{249}Bk	3.40	1.12198	3.79405
^{252}Cf	3.757	0.847458	1.03419

Table 5: Average number of neutrons per fission and Watt parameters for spontaneous fission from Ensslin [12].

1.2 Neutron energy distribution

All of the fission spectra in the Evaluated Nuclear Data Library, ENDL [13] are defined by a simple analytical function, a Watt spectrum defined as

$$W(a, b, E') = C e^{-aE'} \sinh(\sqrt{bE'}) \quad (2)$$

where $C = \sqrt{\pi \frac{b}{4a} \frac{e^{\frac{b}{4a}}}{a}}$, and E' is the secondary neutron energy. The Watt spectrum for ^{235}U and an incident neutron energy of 6 MeV is shown in Fig. 2.

The coefficients a and b vary weakly from one isotope to another and in the case of induced fission, they also vary weakly with the incident neutron energy. For induced fission, b is set identical to 1.0, and a is parametrized as a simple function of the incident neutron energy, as implemented in TART [14, 15]. The fissioning isotope and incident neutron energy determine the value of a , and the energy E' of the secondary neutron emitted is sampled using the Los Alamos' Monte Carlo sampler attributed to Mal Kalos [16].

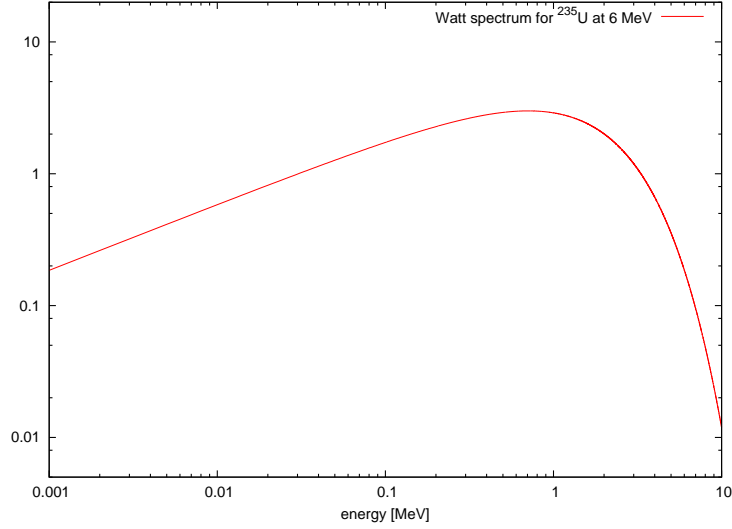


Figure 2: Watt spectrum for ^{235}U and an incident neutron energy of 6 MeV.

For spontaneous fission, the parameters a and b are taken from Ensslin [12] and are listed in Table 5. For spontaneous fission of ^{236}Pu , there is no data for the Watt fission spectrum. We made the assumption that ^{236}Pu has the same Watt fission spectrum as ^{237}Np since they have approximately the same $\bar{\nu}$ (2.07 versus 2.05). We think this is a good approximation since Cullen [15] showed that the Watt fission spectra for neutron-induced fissions can very well be approximated with the single parameter a by setting b equal to 1, instead of the 2 parameters a and b . Since there is only 1 parameter characterizing a Watt spectrum, Watt spectra with identical $\bar{\nu}$'s must have the same value for that parameter a (that is because the integral of the spectrum with respect to the energy gives $\bar{\nu}$, within a normalization factor). If we assume that Watt spectra can be approximated by a single parameter a for spontaneous fissions as well (which we verified and seems to be a valid assumption), there can only be a single Watt spectrum for a given spontaneous fission $\bar{\nu}$. I thus concluded that the Watt spectrum for ^{236}Pu should be close to the Watt spectrum for ^{237}Np and used the Watt parameters of ^{237}Np for ^{236}Pu .

The Watt spectrum is used for all isotopes except ^{252}Cf , for which a special treatment summarized by Valentine [6] is applied. The neutron spectrum for ^{252}Cf is sampled from the Mannhart [17] corrected Maxwellian distribution, the Madland and Nix [18] or the Watt fission spectra from Froehner [19]. These options are selected by the internal variable `neng=0 (default)`, `1`, `2` respectively. The Mannhart distribution is used by default.

The user can choose from three different methods of handling the correlations between neutron energies in a single fission event:

1. Neutron energies are all sampled independently, so there is no explicit energy conservation.
2. A total event energy constraint is imposed in the following way. Beck et al. [20] calculated the average total fission neutron lab kinetic energy as a function of incoming neutron energy E_n for the following 3 isotopes based on the Los Alamos Madland-Nix model [21]:

$$\begin{aligned}
\langle E_{neutron}^{tot} \rangle &= 4.838 + 0.3004E_n & ^{235}\text{U} \\
\langle E_{neutron}^{tot} \rangle &= 4.558 + 0.3070E_n & ^{238}\text{U} \\
\langle E_{neutron}^{tot} \rangle &= 6.128 + 0.3428E_n & ^{239}\text{Pu}
\end{aligned} \tag{3}$$

The fission module uses these average values of the kinetic energies as the mean total neutron energy available to the emission of neutrons. For each fission reaction, the total fission neutron energy $E_{neutron}^{tot}$ is sampled from a normal distribution of mean $\langle E_{neutron}^{tot} \rangle$ and of standard deviation equal to $\langle E_{neutron}^{tot} \rangle / 8$. The numbers of neutrons N is then sampled from the number multiplicity distributions above, and the Watt spectrum is sampled N times to get the energy of these N neutrons. The sampled neutron energies are then rescaled in such a way that the sum of their energies is equal to $E_{neutron}^{tot}$. One of the limitations of this second approach is that it works only for induced fission and for the following 3 isotopes: ^{235}U , ^{238}U and ^{239}Pu .

3. A total event energy constraint is imposed by a method different than that of option 2 above. In 2008, Vogt [22] extended the above Beck et al. [20] method to all actinides, major and minor, in the Evaluated Nuclear Data Library 2008 release, ENDL2008, using data from ENDL2008 and ENDL99. In this extension, the average outgoing prompt gamma energy and prompt neutron energy are expressed by a quadratic expression of the form

$$\langle E_{n/p}^{tot}(E_n) \rangle = c_{n/p} + b_{n/p}E_n + a_{n/p}E_n^2 \tag{4}$$

where the 3 coefficients are actinide-dependent. The coefficients of this quadratic form for prompt fission neutrons are given for 73 actinides in table 6.

1.3 Gamma-ray number distribution

The fission module uses Brunson [23]'s double Poisson model for the spontaneous fission gamma ray multiplicity of ^{252}Cf (see Fig. 3).

$$\Pi(G) = 0.682 \frac{7.20^G e^{-7.20}}{G!} + 0.318 \frac{10.71^G e^{-10.72}}{G!} \tag{5}$$

where G is the gamma ray multiplicity.

The prompt gamma ray multiplicity ranges from 0 to 20 gamma rays per fission with an average of 8.32 gamma rays per fission. This model is a fit to experimental data measured by Brunson himself.

For other isotopes, there is no data available for the multiplicity of prompt gamma rays. Valentine [24] used an approximation that was adopted by the fission module. The probability of emitting G fission gamma rays obeys the negative binomial distribution:

$$\Pi(G) = \binom{\alpha + G - 1}{G} p^G (1 - p)^{\alpha} \tag{6}$$

where the parameter p can be written as $p = \frac{\alpha}{\alpha + \bar{G}}$, α is approximately 26 and \bar{G} is the average number of gamma rays per fission. \bar{G} is approximated by

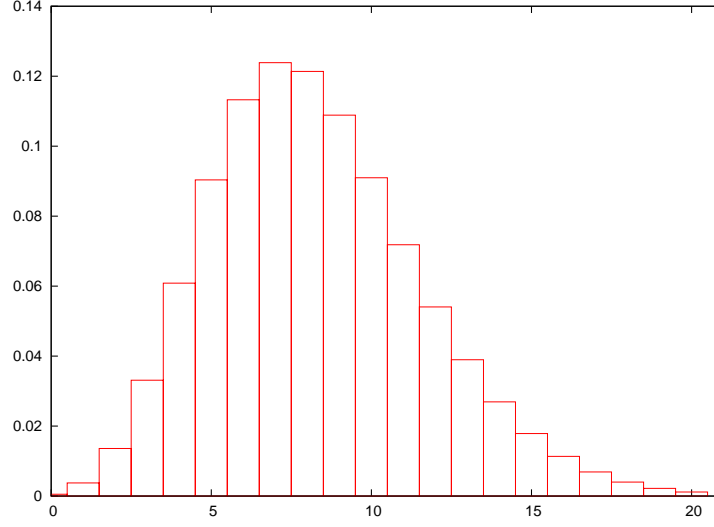


Figure 3: Fission gamma-ray multiplicity for ^{252}Cf .

$$\bar{G} = \frac{E_t(\bar{\nu}, Z, A)}{\bar{E}} \quad (7)$$

where $E_t(\bar{\nu}, Z, A) = (2.51(\pm 0.01) - 1.13 \cdot 10^{-5}(\pm 7.2 \cdot 10^{-8})Z^2\sqrt{A})\bar{\nu} + 4.0$ is the total prompt gamma ray energy, and $\bar{E} = -1.33(\pm 0.05) + 119.6(\pm 2.5)\frac{Z^{\frac{1}{3}}}{A}$ is the average prompt gamma ray energy, and $\bar{\nu}$ is the average number of prompt neutrons. The multiplicity distribution for the spontaneous fission of ^{238}U is shown in Fig. 4.

These multiplicity distributions are only estimates and are not measured data. The fission module uses this model for estimating the number of gamma rays from both spontaneous and induced fission. Note that the energy dependance of the gamma multiplicity for neutron induced fission enters through the parameter $\bar{\nu}$, which is calculated by the parent transport code for the specified isotope.

1.4 Gamma-ray energy distribution

The fission module implements Valentine's [6] model for the energy spectra of fission gamma-rays. The only measured energy spectra for fission gamma-rays are for the spontaneous fission of ^{252}Cf and for the thermal-neutron-induced fission of ^{235}U . Both spectra are similar [25]. Because the ^{235}U measurements are more precise, this data will be used for the fission gamma-ray spectrum. The energy spectrum of the prompt fission gamma rays is obtained from Maienschein's measurements [26] [27]:

$$N(E) = \begin{cases} 38.13(E - 0.085)e^{1.648E} & E < 0.3 \text{ MeV} \\ 26.8e^{-2.30E} & 0.3 < E < 1.0 \text{ MeV} \\ 8.0e^{-1.10E} & 1.0 < E < 8.0 \text{ MeV} \end{cases} \quad (8)$$

This probability function is shown in Fig. 5. Because gamma ray energy spectra are not available, the spectrum above is used for all isotopes, both for spontaneous and induced fission.

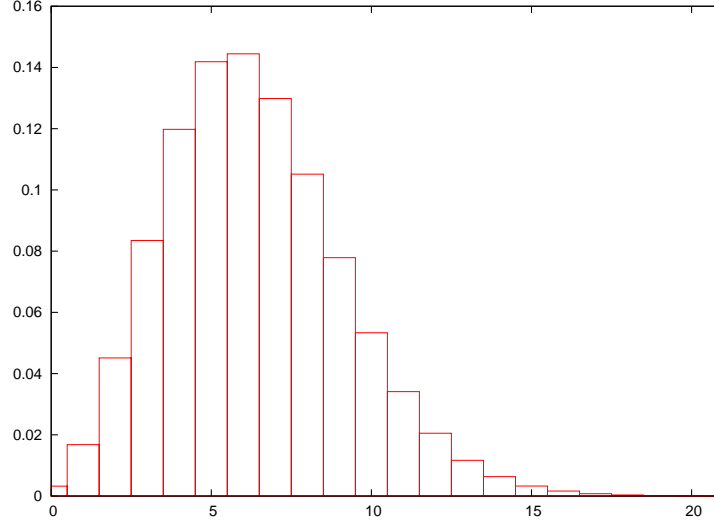


Figure 4: Fission gamma-ray multiplicity for spontaneous fission of ^{238}U .

Regarding the correlation between the energies of gamma-rays emitted by fission reactions, there are three different ways of sampling their energies, as in the case of the fission neutrons. Gamma-ray energies are either all sampled independently (first method), or in such a manner that the total fission gamma-ray energy is bound using an energy conservation principle. Beck et al. [20] computed the average total fission gamma-ray energy to be:

$$\begin{aligned}
 \langle E_{\gamma}^{tot} \rangle &= 6.600 + 0.0777E_n & ^{235}\text{U} \\
 \langle E_{\gamma}^{tot} \rangle &= 6.680 + 0.1239E_n & ^{238}\text{U} \\
 \langle E_{\gamma}^{tot} \rangle &= 6.741 + 0.1165E_n - 0.0017E_n^2 & ^{239}\text{Pu}
 \end{aligned} \tag{9}$$

For each fission reaction, the total fission gamma-ray energy E_{γ}^{tot} is sampled from a normal distribution of mean $\langle E_{\gamma}^{tot} \rangle$ and of standard deviation $\langle E_{\gamma}^{tot} \rangle / 8$. The number of gammas G is then sampled from the number multiplicity distributions above, and the gamma-ray spectrum is sampled G times. The sampled gamma-ray energies are then rescaled in such a way that the sum of their energies is equal to E_{γ}^{tot} . This is the second method of sampling the gamma-ray energies.

The third method is similar to the second one described above for sampling the neutron energies and is based on Vogt [22]. The average outgoing prompt gamma energy is expressed by Eq. 4 where the 3 coefficients are given in table 7. It applies to all major and minor actinides, but since there is data for just a few few actinides in ENDL, most actinides use a generic set of coefficients.

There is a significant discrepancy between the average prompt gamma-ray energies observed using the second and third method, this difference is explained in detail in Vogt [22].

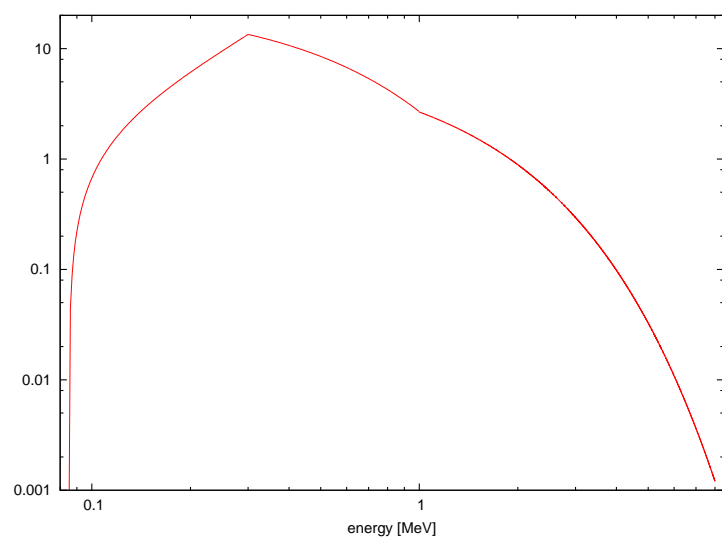


Figure 5: Fission gamma-ray spectrum for ^{235}U .

Actinide	c_n (MeV)	b_n	a_n (MeV ⁻¹)	Actinide	c_n (MeV)	b_n	a_n (MeV ⁻¹)
²²⁵ Ac	3.478	0.1937	-0.001317	²³⁹ Pu	6.092	0.3707	-0.002495
²²⁶ Ac	3.635	0.1231	0.004442	²⁴⁰ Pu	5.906	0.2477	0.008608
²²⁷ Ac	3.396	0.1888	-0.000144	²⁴¹ Pu	6.161	0.2356	0.009310
²²⁷ Th	4.275	0.1225	0.006569	²⁴² Pu	5.926	0.2192	0.008356
²²⁸ Th	3.787	0.2181	0.003449	²⁴³ Pu	5.781	0.4692	0.005751
²²⁹ Th	4.216	0.1339	0.006267	²⁴⁴ Pu	5.655	0.2557	0.008807
²³⁰ Th	3.847	0.1422	0.007380	²⁴⁶ Pu	5.145	0.3155	0.007922
²³¹ Th	4.095	0.1196	0.006487	²⁴⁰ Am	7.150	0.3473	0.002294
²³² Th	3.401	0.3465	-0.000431	²⁴¹ Am	6.957	0.4243	-0.004504
²³³ Th	3.736	0.2566	0.000663	²⁴² Am	7.150	0.3473	0.002294
²³⁴ Th	3.387	0.2290	0.003476	²⁴³ Am	7.422	0.3523	-0.002387
²²⁹ Pa	4.605	0.1744	0.005433	²⁴⁴ Am	6.543	0.3837	0.0
²³⁰ Pa	4.720	0.1879	0.005562	²⁴⁰ Cm	7.525	0.2786	0.011040
²³¹ Pa	4.524	0.1726	0.006436	²⁴¹ Cm	7.699	0.3648	0.007316
²³² Pa	4.699	0.1683	0.006763	²⁴² Cm	7.701	0.2683	0.011400
²³³ Pa	4.076	0.3671	0.000639	²⁴³ Cm	8.104	0.2363	0.005492
²³⁰ U	4.977	0.1832	0.006792	²⁴⁴ Cm	7.103	0.2061	0.010830
²³¹ U	5.196	0.2127	0.005808	²⁴⁵ Cm	7.984	0.2279	0.005426
²³² U	6.082	0.2782	0.003243	²⁴⁶ Cm	6.939	0.2245	0.009390
²³³ U	5.141	0.2540	0.002915	²⁴⁷ Cm	8.216	0.3896	0.008595
²³⁴ U	4.728	0.2339	0.002704	²⁴⁸ Cm	7.295	0.2499	0.013550
²³⁵ U	4.864	0.3114	-0.001424	²⁴⁹ Cm	7.124	0.3777	0.008907
²³⁶ U	4.505	0.2969	0.004555	²⁵⁰ Cm	6.973	0.4062	0.006831
²³⁷ U	4.999	0.2680	0.001783	²⁴⁵ Bk	8.210	0.3643	0.009615
²³⁸ U	4.509	0.3574	-0.004351	²⁴⁶ Bk	8.274	0.4764	0.005445
²³⁹ U	4.580	0.3647	0.004266	²⁴⁷ Bk	7.831	0.4266	0.008129
²⁴⁰ U	4.561	0.3596	0.000273	²⁴⁸ Bk	8.145	0.4796	0.006656
²⁴¹ U	4.268	0.3998	0.002821	²⁴⁹ Bk	7.519	0.4021	0.010130
²³⁴ Np	5.880	0.2311	0.007642	²⁵⁰ Bk	7.879	0.4204	0.008308
²³⁵ Np	5.576	0.2484	0.007751	²⁴⁶ Cf	8.900	0.4323	0.009000
²³⁶ Np	5.080	0.2446	0.008116	²⁴⁸ Cf	8.661	0.3877	0.010700
²³⁷ Np	5.330	0.2768	0.005819	²⁴⁹ Cf	9.428	0.4746	0.007067
²³⁸ Np	5.214	0.2650	0.007559	²⁵⁰ Cf	8.226	0.4980	0.007397
²³⁹ Np	5.416	0.2489	0.004159	²⁵¹ Cf	9.407	0.4454	0.010790
²³⁶ Pu	6.112	0.2240	0.009279	²⁵² Cf	8.627	0.5190	0.007184
²³⁷ Pu	6.177	0.2599	0.006790	²⁵³ Cf	8.449	0.2396	0.018650
²³⁸ Pu	6.087	0.2189	0.008211				

Table 6: Coefficients of Eq. 4 for the energy-dependent average outgoing prompt fission neutron energy.

Actinide	c_p (MeV)	b_p	a_p (MeV ⁻¹)
²³² U	7.256	0.0255	0.000182
²³⁵ U	7.284	0.2295	-0.00474
²³⁸ U	6.658	0.01607	-1.22e-7
²³⁹ Pu	6.857	0.4249	-0.009878
²⁵² Cf	6.44186	0.01831	0.
generic	6.95	0.01693	7.238e-8

Table 7: Coefficients of Eq. 4 for the energy-dependent average outgoing prompt fission photon energy.

2 User manual

This section describes how to use the general-purpose and extensible software library libFission.a to accurately simulate neutron and gamma-ray emission from fission. The first section describes the fission library interface, the next three sections describe how to run the three popular Monte-Carlo particle transport codes MCNPX [28], Geant4 [29] [30] and COG, using the fission library to sample the fission neutrons and gamma-rays. The standalone version of the software library can be downloaded from <http://nuclear.llnl.gov/CNP/simulation>.

2.1 Limitations of the fission library

The range of neutron energies for which induced fission neutron multiplicity data were available in the literature spans the range from 0 to 10 MeV, to which corresponds a range of $\bar{\nu}$ values. The sampling of number of neutrons per fission is based on either the incident neutron energy or the nubar corresponding to that energy (depending on the option selected in *setnudist*). When sampling is based on the energy, the neutron multiplicity data at 10 MeV is used for incident neutron energies greater than 10 MeV. This is clearly incorrect, and sampling based on nubar is therefore preferred. When sampling is based on nubar, and the nubar is in the range for which we have multiplicity data from the literature, that data is used. Outside that range, Terrell approximation is used. Sampling based on nubar is the default for the fission module.

In the case of spontaneous fission, data is only available for the following isotopes: ^{232}Th , ^{232}U , ^{233}U , ^{234}U , ^{235}U , ^{236}U , ^{238}U , ^{237}Np , ^{238}Pu , ^{239}Pu , ^{240}Pu , ^{241}Pu , ^{242}Pu , ^{241}Am , ^{242}Cm , ^{244}Cm , ^{249}Bk , and ^{252}Cf . The 3 Monte-Carlo MCNPX, COG and Geant4 do not emit any particles if a different spontaneous fission isotope is specified.

2.2 Fission library interface

The interface to the fission library consists of 22 C functions, each of which will be described below:

void genspfissevt_(int *isotope, double *time)

This function is called to trigger a spontaneous fission. Multiple neutrons and gamma-rays are generated and stored in a stack along with their energies, directions and emission times. The arguments of this function are

isotope: entered in the form ZA (e.g. 94239 for ^{239}Pu)

time: the time of the spontaneous fission

The generated neutrons and gamma-rays, along with their properties will be lost upon the next call to genspfissevt_ or genfissevt_. Therefore, they must be retrieved immediately by the caller using the appropriate functions described below.

void genfissevt_(int *isotope, double *time, double *nubar, double *eng)

This function is called to trigger a neutron-induced fission. In addition to the arguments above, the fission inducing neutron is characterized by:

nubar: user-specified average number of neutrons emitted per fission (e.g. as tabulated in the cross-section libraries used by the particle transport code)
eng: energy of the neutron inducing fission

Either the average number $\bar{\nu}$ of neutrons emitted per fission or the energy *eng* of the fission inducing neutron will be used to determine the number of neutrons sampled, see function 2.2 below. On the other side, the number of gamma-rays sampled only depends on $\bar{\nu}$. As for genspfissevt_, the generated neutrons and gamma-rays are lost upon subsequent calls to genspfissevt_ and genfissevt_.

int getnnu_() and int getpnu_()

These functions return the numbers of neutrons and gamma-rays emitted in the fission reaction, or -1 if no number could be sampled in the fission library due to lack of data. The reader is referred to the physics reference manual to find the list of isotopes for which sampling will return positive numbers.

double getneng_(int *index) and double getpeng_(int *index) double getnvel_(int *index) and double getpvel_(int *index)

These functions return the energies and velocities of the neutrons/gamma-rays.

double getndircosu_(int *index), double getndircosv_(int *index), double getndircosw_(int *index)

double getpdircosu_(int *index), double getpdircosv_(int *index), double getpdircosw_(int *index)

These 2 families of functions return the direction cosines of the velocity vector on the x, y and z axes for the fission neutrons and gamma-rays.

double getnage_(int *index) and double getpage_(int *index)

This functions returns the age of the fission neutron/gamma-ray, or -1 if index is out of range. The age returned might be different from the time specified in genfissevt_ and genspfissevt_ for delayed neutrons and gamma-rays, see function setdelay_ 2.2 below. Currently, delayed fission neutrons/gamma-rays are not implemented, so all fission products are emitted promptly.

void setdelay_(int *delay)

This function is called to enable delayed neutrons and gamma-rays. The argument *delay* is set to

- 0 (default) for strictly prompt neutrons and photons
- 1 (n/a) for prompt neutrons, prompt and delayed photons
- 2 (n/a) for prompt and delayed neutrons, prompt photons
- 3 (n/a) for prompt and delayed neutrons, prompt and delayed photons

Delayed neutrons and gamma-rays have not yet been implemented in the fission library. This setting has presently no effect on the age sampling. All neutrons and photons are currently emitted promptly (delay=0).

void setcorrel_(int *correlation)

This function is called to set the type of neutron/gamma-ray correlation. The argument *correlation* is set to

- 0 (default) for no correlation between neutrons and photons
- 1 total fission neutron energy and total fission gamma-ray energy are sampled from normal distributions of means given in Beck et al. [20]. No correlation between the number of neutrons and the number of gamma-rays
- 2 total fission neutron energy and total fission gamma-ray energy are sampled from normal distributions of means given in Vogt [22]. No correlation between the number of neutrons and the number of gamma-rays
- 3 (n/a) for number and energy correlation between neutrons and photons

void setnudist_(int *nudist)

This selects the data to be sampled for the neutron number distributions for neutron-induced fission. If there is no data available, then in all cases the Terrell approximation is used. The argument *nudist* can take 3 values:

- 0 Use the fit to the Zucker and Holden tabulated P_v distributions as a function of energy for ^{235}U , ^{238}U and ^{239}Pu .
- 1 Use fits to the Zucker and Holden tabulated P_v distribution as a function of energy for ^{238}U and ^{239}Pu , and a fit to the Zucker and Holden data as well as the Gwin, Spencer and Ingle data (at thermal energies) as a function of energy for ^{235}U .
- 2 Use the fit to the Zucker and Holden tabulated P_v distributions as a function of \bar{v} . The ^{238}U fit is used for the ^{232}U , ^{234}U , ^{236}U and ^{238}U isotopes, the ^{235}U fit for ^{233}U and ^{235}U , the ^{239}Pu fit for ^{239}Pu and ^{241}Pu .
- 3 (default) Use the discrete Zucker and Holden tabulated P_v distributions and corresponding \bar{v} s. Sampling based on the incident neutron \bar{v} . The ^{238}U data tables are used for the ^{232}U , ^{234}U , ^{236}U and ^{238}U isotopes, the ^{235}U data for ^{233}U and ^{235}U , the ^{239}Pu data for ^{239}Pu and ^{241}Pu .

void setcf252_(int *ndist, int *neng)

This function is specific to the spontaneous fission of ^{252}Cf . It selects the data to be sampled for the neutron number and energy distributions and takes the following arguments:

- ndist: Sample the number of neutrons
 - 0 (default) from the tabulated data measured by Spencer
 - 1 from Boldeman's data
- neng: Sample the spontaneous fission neutron energy
 - 0 (default) from Mannhart corrected Maxwellian spectrum
 - 1 from Madland-Nix theoretical spectrum
 - 2 from the Froehner Watt spectrum

void setrngf_(float (*funcptr) (void)) and void setrngd_(double (*funcptr) (void))

This function sets the random number generator to the user-defined one specified in the argument. If either setrngf_ or setrngd_ are not specified, the default system call srand48 is used. The arguments are random number generator functions that returns variables of type float and double respectively.

2.3 Geant4

This physics module is now part of the Geant4 distribution as of release 4.9.0. Instructions on how to add this library by hand in earlier versions is described below.

Compilation

Please refer to the `geant` directory in the fission library source code distribution for a complete example and explicit instructions for compiling and linking the fission library with Geant4. Besides setting the usual environmental variables for Geant4, one also needs to set `EXTRALIBS` to `-lfission` before building the executable. The fission library `libFission.a` must be located in a directory specified in the link line. A good place for `libFission.a` is the directory `$G4WORKDIR/tmp/$G4SYSTEM/exec_name`. The header file `Fission.hh` must be in the include directory.

Execution

The environment variable *NeutronHPCrossSections* must point to the G4NDL3.10 directory, where the induced fission cross-sections and data are located.

Limitations

The induced-fission data available in G4NDL3.10 is scarce. At the time of this writing, there are only data files for 7 isotopes of Uranium: ^{232}U , ^{233}U , ^{234}U , ^{235}U , ^{236}U , ^{237}U and ^{238}U . The origin of the data has not been investigated. For other isotopes, induced fission will not emit any particles. The fission library does not have any spontaneous fission data for isotopes other than the ones listed in section 2.1.

Description of c++ classes

For neutron induced fission, this model is intended to be used with the low energy neutron interaction data libraries with class *G4Fisslib* specified in the physics list as the *G4HadronFissionProcess* instead of class *G4NeutronHPFission*. Here is an example code snippet for registering this model in the physics list:

```
G4ProcessManager* pmanager = particle->GetProcessManager();
G4String particleName = particle->GetParticleName();

if (particleName == "gamma") {
    (...)
} else if (particleName == "neutron") {
    (...)
    // Fission library model
    G4HadronFissionProcess *theFissionProcess = new G4HadronFissionProcess();
    G4FissLib* theFissionModel = new G4FissLib;
    theFissionProcess->RegisterMe(theFissionModel);
    pmanager->AddDiscreteProcess(theFissionProcess);
    (...)
} else ...
```

The constructor of *G4FissLib* does two things. First it reads the necessary fission cross-section data in the file located in the directory specified by the environment variable *NeutronHPCrossSections*. It does this by initializing one object of class *G4NeutronHPChannel* per isotope present in the geometry. Second, it registers an instance of *G4FissionLibrary* for each isotope as the model for that reaction/channel. When Geant4 tracks a neutron to a reaction site and the fission library process is selected among all other process for neutron reactions, the method *G4FissLib::ApplyYourself* is called, and one of the fissionable isotopes present at the reaction site is selected. This method in turn calls *G4NeutronHPChannel::ApplyYourself* which calls *G4FissionLibrary::ApplyYourself*, where the induced neutrons and gamma-rays are emitted by sampling the fission library.

For spontaneous fission the user must provide classes *PrimaryGeneratorAction*, *MultipleSource*, *MultipleSourceMessenger*, *SingleSource*, *SponFissIsotope* to generate spontaneous fission neutrons and gammas. Examples of these classes can be downloaded from <http://nuclear.llnl.gov/CNP/simulation>. Spontaneous fissions are generated in the *PrimaryGeneratorAction* class. The spontaneous fission source needs to be described in terms of geometry, isotopic composition and fission strength. Once this information is given, the constructor creates as many spontaneous fission isotopes of class *SponFissIsotope* as specified, and adds them to the source of class *MultipleSource*. When Geant needs to generate particles, it calls the method *PrimaryGeneratorAction::GeneratePrimaries*, which first sets the time of the next fission based on the fission rates entered in the constructor, and then calls the method *MultipleSource::GeneratePrimaryVertex* which determines which one of the spontaneous fission isotopes will fission. This method in turn calls the method *SponFissIsotope::GeneratePrimaryVertex* for the chosen isotope. It is in this method that the neutrons and photons sampled from the fission library are added to the stack of secondary particles. Sources other than spontaneous fission isotopes can be added to the source of class *MultipleSource*. For instance, a background term emitting a large number of background gamma-rays can be added, as long as it derives from the class *SingleSource*. The intensity of that source would be set the same way as for the spontaneous fission isotope sources.

2.4 MCNPX

This physics module has been submitted to the MCNPX development team and will appear in a future release. The fission physics included in the library libFission.a is readily available to MCNPX users via a flag on the PHYS:N card. To enable sampling of neutrons and gamma-rays from libFission.a, the 6th entry *fism* of the PHYS:N card should be set to 5:

```
phys:n 100 0 0 -1 -1 5
```

fism=5 is the only MCNPX setting for which gamma-rays are sampled in analog for fission reactions. The fission library can be sampled for both induced and spontaneous fission reactions, the latter only when the *par* flag of the source definition card *sdef* is set to *sf*:

```
sdef par=sf
```

as to specify a spontaneous fission source in MCNPX. In the case of spontaneous fissions, only the isotopes listed above in section 2.1 have data in the fission library. For other spontaneous fission isotopes, no neutrons, nor gamma-rays are emitted.

This *fism* setting has an effect on the standard MCNPX gamma production sampling. By default, MCNPX emits a number of gamma-rays at each neutron collision site, independent of the type of nuclear reaction. This number is sampled from an energy dependent photon yield curve, which is the sum of the production yields from different nuclear reactions. While this method is not accurate on a per reaction basis, this leads to the right number of gammas emitted on average. When this fission library is active (*fism*=5) the contribution to the photon yield curve that corresponds to fission reactions is suppressed so that the total average number of gamma rays produced is correct.

2.5 COG

This physics module has been submitted to the COG development team and will appear in a future release. The fission library libFission.a can be sampled for induced fissions in COG using the *FISSLIB* keyword in the MIX block of the input deck. This is not the default. The *NUOPTION* can not be used concurrently, it is not compatible with *FISSLIB*.

COG is similar to MCNPX in that it emits a number of gamma-rays at each neutron collision site, and this number is independent on the reaction type. The keyword *NOGAMPRO* can be used to completely turn off this gamma-ray production.

Spontaneous fissions are implemented using a COG user source. A sample user source 'spfiss.F' is available in the COG distribution subdirectory 'usrsrc'. Compiling a COG user source is trivial:

```
make -f COGUserlib.make in=spfiss.F
```

Using the right compiler at compile time is important, and if this becomes an issue, a COG developer should be contacted. It is also important to use a COG version that is compatible with user sources and user detectors. Not all COG versions work with user sources/detectors.

An example of input deck using the 'spfiss' spontaneous fission source is located in the 'usrsrc' directory. The important lines related to the user source are in the SOURCE block:

```
SOURCE
NPART = 5e4  $ NPART is the sum of spontaneous fission neutrons and photons
$
$ The source below is for a HEU shell (93% enriched in U-235).
$ We neglect here the spontaneous fissions in U-235. The fission rate
$ for 350 g of U-238 is 350[g]*1.36*10E-2[n/g/s] = 4.76 n/s. With
$ spontaneous nubar equal to 2.01, we have
$ 4.76[n/s]/2.01[n/fission] = 2.368 fissions/sec
$
$      name      isotope  strength  xcenter  ycenter  zcenter  Rin  Rout  FissRate
$      (1)      (2)      (3)      (4)      (5)      (6)  (7)  (8)
USRSOR spfiss  92238    1.        0.        0.        0.        1.  3.96  2.368
$
```

NPART is the sum of all source particles, that is both spontaneous fission neutrons and gamma-rays. The line USRSOR has several arguments: The argument under 'name' specify the FORTRAN subroutine to be used a the spontaneous fission source: 'spfiss'. The first numeric argument is the isotope in the form ZA, followed by the source strength (not relevant in this case), the center of the shell (x, y, z), the inner and outer radii and the fission rate in fissions/second. Note the units of the fission rate, fissions/second and not neutrons/second.

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